



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:52 AM UTC

PDB ID : 5IE4 / pdb_00005ie4
Title : Crystal structure of a lactonase mutant in complex with substrate a
Authors : Zheng, Y.Y.; Xu, Z.X.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2016-02-25
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

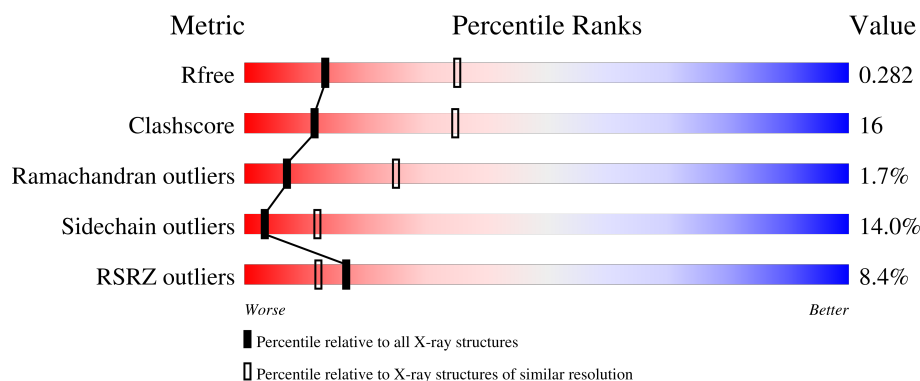
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	2% 67% 27% 6%
1	B	264	2% 73% 23% ..
1	C	264	18% 26% 23% 7% 43%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5445 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

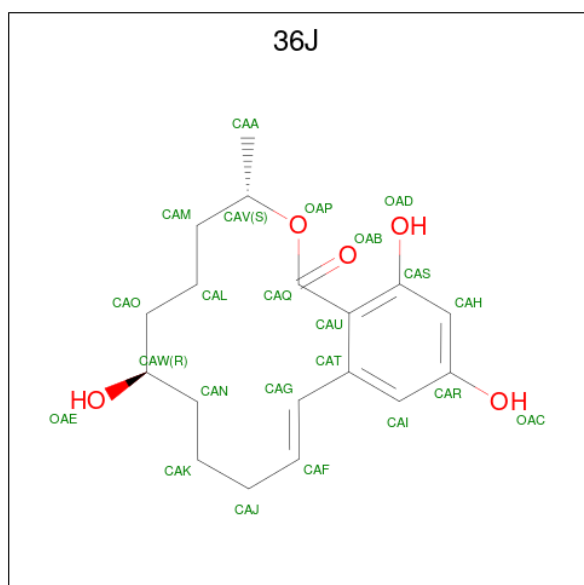
- Molecule 1 is a protein called Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2020	1282	341	386	11			
1	B	264	Total	C	N	O	S	0	0	0
			2020	1282	341	386	11			
1	C	151	Total	C	N	O	S	0	0	0
			1159	744	191	216	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	SER	engineered mutation	UNP Q8NKB0
B	102	ALA	SER	engineered mutation	UNP Q8NKB0
C	102	ALA	SER	engineered mutation	UNP Q8NKB0

- Molecule 2 is (3S,7R,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (CCD ID: 36J) (formula: C₁₈H₂₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		

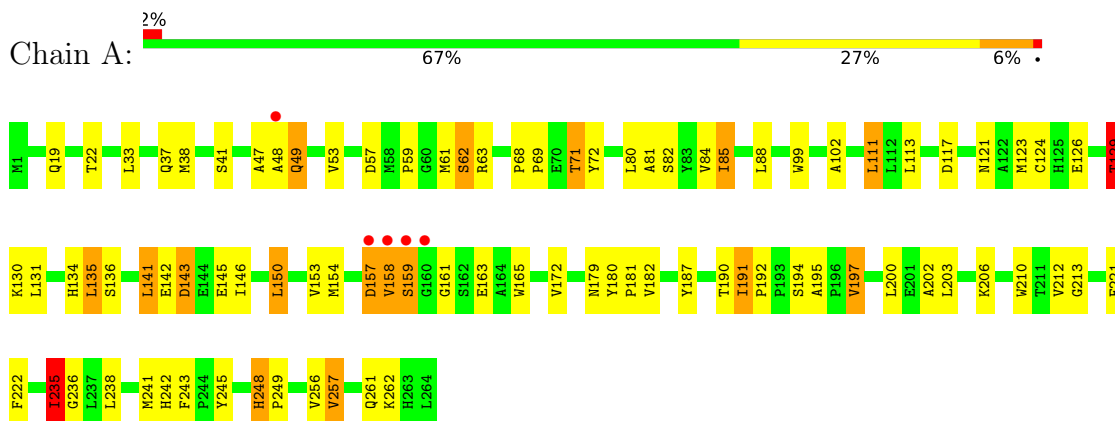
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	76	Total	O	0	0
			76	76		
3	C	54	Total	O	0	0
			54	54		

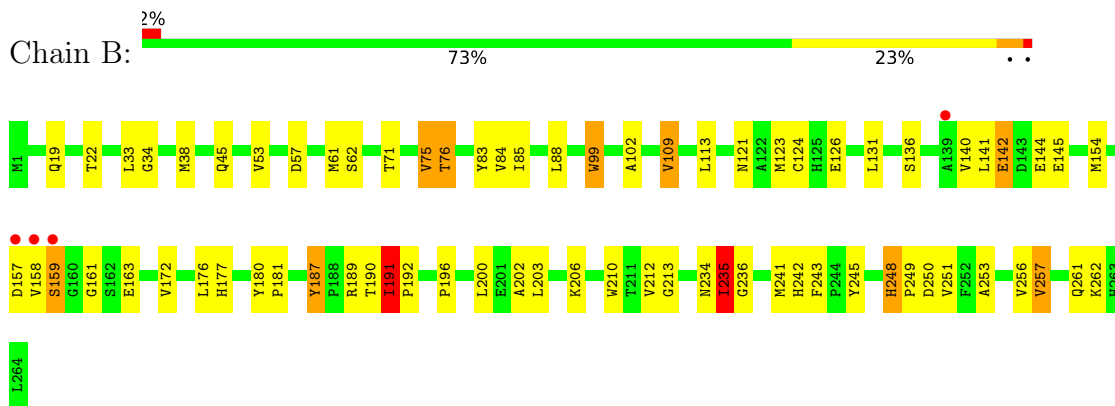
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

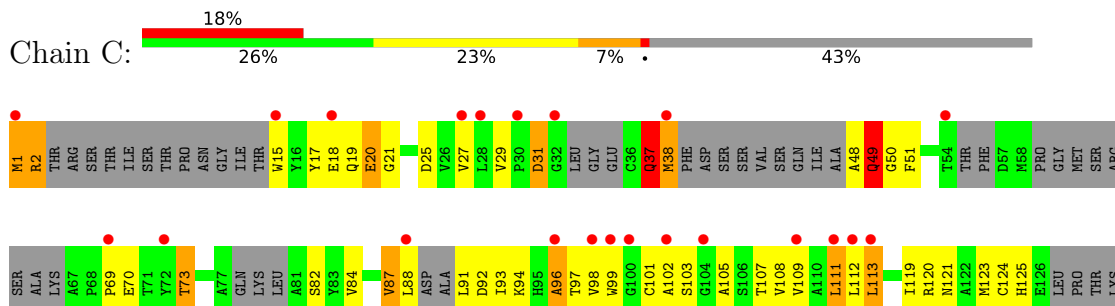
- Molecule 1: Zearalenone hydrolase

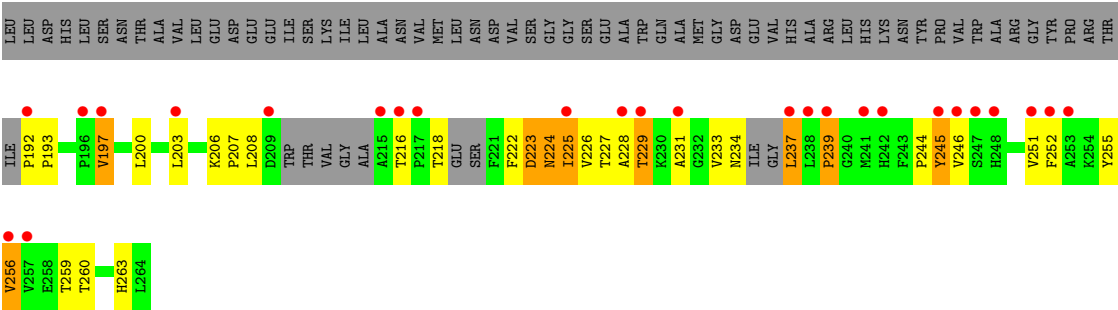


- Molecule 1: Zearalenone hydrolase



- Molecule 1: Zearalenone hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 86.20Å 473.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (25.00-2.80) 97.6 (25.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.96 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.203 , 0.265 0.230 , 0.282	Depositor DCC
R_{free} test set	1264 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5445	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 36J

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	0/2071	1.04	8/2829 (0.3%)
1	B	0.75	0/2071	1.02	6/2829 (0.2%)
1	C	0.71	0/1181	0.92	1/1599 (0.1%)
All	All	0.74	0/5323	1.01	15/7257 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	7
All	All	0	11

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ILE	CA-C-N	-7.62	112.53	120.38
1	B	191	ILE	C-N-CA	-7.62	112.53	120.38
1	A	49	GLN	N-CA-C	-7.18	98.61	109.60
1	A	248	HIS	CA-C-N	6.28	125.50	118.97
1	A	248	HIS	C-N-CA	6.28	125.50	118.97
1	C	256	VAL	N-CA-C	5.81	115.88	110.42
1	A	158	VAL	N-CA-C	5.72	119.25	113.47
1	A	235	ILE	N-CA-C	5.59	116.79	108.46
1	A	197	VAL	CB-CA-C	5.38	116.03	110.70
1	B	191	ILE	N-CA-CB	5.36	113.88	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	HIS	CA-C-N	5.28	124.46	118.97
1	B	248	HIS	C-N-CA	5.28	124.46	118.97
1	A	197	VAL	N-CA-C	-5.26	108.15	113.20
1	B	235	ILE	N-CA-C	5.26	116.23	108.45
1	A	129	THR	N-CA-C	-5.13	108.04	114.56

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ASP	Peptide
1	B	140	VAL	Peptide
1	B	157	ASP	Peptide
1	B	75	VAL	Peptide
1	C	15	TRP	Peptide
1	C	229	THR	Peptide
1	C	239	PRO	Peptide
1	C	37	GLN	Peptide
1	C	50	GLY	Peptide
1	C	87	VAL	Peptide
1	C	96	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2020	0	1991	62	0
1	B	2020	0	1991	43	0
1	C	1159	0	1132	56	0
2	A	23	0	22	5	0
2	B	23	0	22	7	0
3	A	70	0	0	1	0
3	B	76	0	0	0	0
3	C	54	0	0	1	0
All	All	5445	0	5158	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 16.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:HG22	1:C:233:VAL:O	1.73	0.88
1:B:158:VAL:HG22	1:B:242:HIS:HB2	1.63	0.81
1:C:239:PRO:HG3	1:C:251:VAL:HG11	1.64	0.79
1:B:75:VAL:HG12	1:B:76:THR:H	1.46	0.79
1:A:158:VAL:HB	1:A:242:HIS:CD2	2.19	0.78
1:C:38:MET:HG2	1:C:246:VAL:HG22	1.65	0.78
1:A:59:PRO:CB	1:A:71:THR:CG2	2.62	0.77
1:A:59:PRO:HB2	1:A:71:THR:CG2	2.15	0.77
1:C:1:MET:O	1:C:20:GLU:OE1	2.05	0.75
1:A:142:GLU:C	1:A:143:ASP:O	2.29	0.73
1:C:120:ARG:HD2	1:C:263:HIS:O	1.89	0.73
1:B:38:MET:HE2	1:B:245:TYR:HE1	1.56	0.71
1:A:38:MET:HE2	1:A:245:TYR:HE1	1.56	0.69
1:A:59:PRO:HB3	1:A:71:THR:CG2	2.24	0.68
1:C:19:GLN:O	1:C:20:GLU:HB2	1.92	0.68
1:A:142:GLU:O	1:A:143:ASP:O	2.14	0.66
1:C:239:PRO:CG	1:C:251:VAL:HG11	2.26	0.66
1:A:59:PRO:HB3	1:A:71:THR:HG21	1.79	0.65
1:C:87:VAL:O	1:C:91:LEU:N	2.30	0.64
1:C:105:ALA:O	1:C:108:VAL:HG22	1.96	0.64
1:A:47:ALA:O	1:A:49:GLN:O	2.15	0.64
1:C:121:ASN:HA	1:C:207:PRO:HB2	1.79	0.64
1:A:38:MET:HE1	1:A:243:PHE:CD1	2.34	0.63
1:C:84:VAL:HG11	1:C:111:LEU:HD21	1.81	0.62
1:C:101:CYS:SG	1:C:102:ALA:N	2.69	0.62
1:B:38:MET:HE1	1:B:243:PHE:CD1	2.35	0.61
1:C:69:PRO:O	1:C:73:THR:OG1	2.19	0.60
1:C:21:GLY:HA3	1:C:51:PHE:O	2.02	0.60
1:C:223:ASP:O	1:C:224:ASN:C	2.44	0.59
1:B:75:VAL:HG12	1:B:76:THR:N	2.15	0.58
1:A:57:ASP:CG	1:A:63:ARG:HH21	2.11	0.58
1:A:81:ALA:HB1	1:A:111:LEU:HD13	1.85	0.58
1:B:180:TYR:HB2	1:B:181:PRO:HD3	1.85	0.58
1:C:123:MET:HE1	1:C:256:VAL:HG13	1.85	0.58
1:B:154:MET:HE2	1:B:243:PHE:CZ	2.39	0.58
1:A:68:PRO:O	1:A:71:THR:HB	2.03	0.57
1:C:17:TYR:CD1	1:C:91:LEU:HD21	2.39	0.57
1:A:157:ASP:HB2	1:A:158:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HG	2:B:301:36J:H9	1.88	0.56
1:C:120:ARG:CD	1:C:263:HIS:O	2.54	0.56
1:A:180:TYR:HB2	1:A:181:PRO:HD3	1.88	0.56
1:C:125:HIS:CE1	1:C:244:PRO:HG3	2.40	0.56
2:B:301:36J:H8	2:B:301:36J:OAB	2.07	0.55
1:A:102:ALA:HB1	2:A:300:36J:CAQ	2.37	0.55
1:A:48:ALA:C	1:A:49:GLN:O	2.46	0.55
1:A:59:PRO:CB	1:A:71:THR:HG23	2.37	0.54
1:A:158:VAL:CB	1:A:242:HIS:CD2	2.88	0.54
1:A:248:HIS:N	1:A:249:PRO:HD3	2.22	0.54
1:A:159:SER:HA	1:A:243:PHE:HD2	1.73	0.53
1:A:59:PRO:HB2	1:A:71:THR:HG22	1.89	0.53
1:B:235:ILE:HG13	1:B:236:GLY:N	2.23	0.53
1:C:112:LEU:HD21	1:C:206:LYS:HB3	1.91	0.53
1:C:197:VAL:O	1:C:197:VAL:HG13	2.07	0.53
1:C:218:THR:HG23	1:C:222:PHE:HB2	1.90	0.52
1:C:192:PRO:HB2	1:C:193:PRO:HD3	1.90	0.52
1:A:38:MET:CE	1:A:245:TYR:HE1	2.23	0.52
1:C:252:PHE:CE1	1:C:256:VAL:HG21	2.45	0.52
1:B:158:VAL:HG22	1:B:242:HIS:CB	2.37	0.52
1:A:146:ILE:CG2	1:A:150:LEU:HD22	2.39	0.52
1:B:159:SER:HA	1:B:243:PHE:HD2	1.75	0.52
1:A:134:HIS:CE1	1:A:135:LEU:HD13	2.45	0.51
1:A:142:GLU:O	1:A:143:ASP:C	2.53	0.51
1:C:223:ASP:O	1:C:226:VAL:N	2.43	0.51
1:A:59:PRO:HB2	1:A:71:THR:HG23	1.89	0.51
1:C:92:ASP:C	1:C:93:ILE:HD12	2.35	0.51
1:B:154:MET:HE3	1:B:154:MET:HA	1.92	0.51
1:B:99:TRP:CD1	1:B:99:TRP:C	2.88	0.51
2:B:301:36J:OAB	2:B:301:36J:OAD	2.26	0.51
2:A:300:36J:CAG	2:A:300:36J:OAP	2.55	0.51
1:A:158:VAL:HB	1:A:242:HIS:HD2	1.69	0.51
1:A:257:VAL:HG23	1:A:261:GLN:NE2	2.27	0.50
1:A:61:MET:O	1:A:62:SER:C	2.54	0.50
1:C:208:LEU:HB3	1:C:233:VAL:HG13	1.94	0.50
1:C:228:ALA:HB2	3:C:305:HOH:O	2.11	0.50
1:B:38:MET:CE	1:B:245:TYR:HE1	2.24	0.50
1:C:1:MET:O	1:C:20:GLU:CD	2.54	0.50
1:A:235:ILE:HG13	1:A:236:GLY:N	2.27	0.49
1:C:99:TRP:CE2	1:C:252:PHE:HE2	2.30	0.49
1:C:237:LEU:HD22	1:C:237:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HE1	1:B:256:VAL:HG13	1.94	0.49
1:A:191:ILE:HG22	1:A:192:PRO:CD	2.43	0.49
1:C:97:THR:HG22	1:C:123:MET:HE3	1.94	0.49
1:C:97:THR:HG21	1:C:260:THR:OG1	2.13	0.48
1:A:158:VAL:CB	1:A:242:HIS:HD2	2.25	0.48
1:B:212:VAL:HG12	1:B:213:GLY:N	2.28	0.48
1:B:75:VAL:CG1	1:B:76:THR:H	2.21	0.48
1:B:144:GLU:OE2	1:B:177:HIS:CE1	2.67	0.48
1:A:157:ASP:CB	1:A:158:VAL:HG13	2.44	0.48
1:B:248:HIS:N	1:B:249:PRO:HD3	2.29	0.48
1:A:37:GLN:HG2	1:A:172:VAL:HG22	1.96	0.47
1:A:123:MET:HE1	1:A:256:VAL:HG13	1.95	0.47
2:B:301:36J:H15	2:B:301:36J:OAP	2.14	0.47
1:A:212:VAL:HG12	1:A:213:GLY:N	2.29	0.47
1:B:71:THR:HG22	1:B:83:TYR:CZ	2.49	0.47
2:A:300:36J:OAB	2:A:300:36J:H8	2.14	0.47
1:B:154:MET:CE	1:B:243:PHE:CE2	2.98	0.47
1:C:99:TRP:HE3	1:C:123:MET:HB2	1.79	0.47
1:B:61:MET:O	1:B:62:SER:C	2.58	0.47
1:C:231:ALA:HB3	1:C:233:VAL:HG23	1.97	0.47
1:C:218:THR:CG2	1:C:222:PHE:HB2	2.45	0.46
1:A:99:TRP:CD1	1:A:99:TRP:C	2.94	0.46
1:C:96:ALA:O	1:C:119:ILE:HA	2.15	0.46
1:A:129:THR:HG22	1:A:130:LYS:HG2	1.97	0.46
1:B:124:CYS:HG	1:B:210:TRP:CG	2.34	0.46
1:B:75:VAL:HG21	1:B:187:TYR:CE1	2.50	0.46
1:A:85:ILE:HD13	1:A:85:ILE:HA	1.87	0.45
1:A:158:VAL:HA	1:A:241:MET:HE2	1.97	0.45
1:A:191:ILE:HG22	1:A:192:PRO:HD3	1.98	0.45
1:C:93:ILE:HD12	1:C:93:ILE:N	2.31	0.45
1:B:38:MET:HE1	1:B:243:PHE:CE1	2.52	0.45
1:B:158:VAL:HA	1:B:241:MET:HE2	1.99	0.45
1:C:105:ALA:O	1:C:108:VAL:N	2.44	0.45
1:C:29:VAL:HG11	1:C:107:THR:HG21	1.99	0.45
1:B:191:ILE:HG22	1:B:192:PRO:CD	2.46	0.45
1:A:126:GLU:OE1	1:A:242:HIS:ND1	2.49	0.45
1:A:124:CYS:HG	1:A:210:TRP:CG	2.34	0.45
1:B:126:GLU:OE1	1:B:242:HIS:ND1	2.49	0.45
1:B:142:GLU:HB2	1:B:145:GLU:HB2	1.97	0.45
1:A:117:ASP:OD1	1:A:117:ASP:N	2.49	0.44
1:A:19:GLN:HA	1:A:53:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:SER:O	1:A:195:ALA:C	2.60	0.44
1:C:31:ASP:OD1	1:C:31:ASP:N	2.49	0.44
1:B:141:LEU:O	1:B:142:GLU:HB2	2.17	0.44
1:A:69:PRO:HA	1:A:72:TYR:CZ	2.53	0.44
1:A:80:LEU:O	1:A:84:VAL:HG23	2.18	0.44
1:A:154:MET:HA	1:A:158:VAL:CG2	2.48	0.44
1:B:75:VAL:CG1	1:B:76:THR:N	2.81	0.44
1:B:45:GLN:HE22	1:B:250:ASP:HA	1.83	0.44
1:B:191:ILE:HG22	1:B:192:PRO:HD3	1.99	0.44
1:B:253:ALA:O	1:B:257:VAL:HG13	2.18	0.44
1:A:146:ILE:HG23	1:A:150:LEU:HD22	2.00	0.43
1:A:202:ALA:O	1:A:206:LYS:HE2	2.18	0.43
1:B:102:ALA:HB1	2:B:301:36J:CAQ	2.48	0.43
1:C:97:THR:CG2	1:C:123:MET:HE3	2.47	0.43
1:C:228:ALA:O	1:C:231:ALA:HB3	2.17	0.43
1:C:97:THR:CG2	1:C:123:MET:CE	2.96	0.43
1:A:135:LEU:HD21	2:A:300:36J:H20	2.00	0.43
1:B:154:MET:HE2	1:B:243:PHE:HZ	1.81	0.43
1:C:225:ILE:H	1:C:225:ILE:HG13	1.51	0.43
1:A:38:MET:HE1	1:A:243:PHE:CE1	2.54	0.43
1:A:141:LEU:HG	1:A:145:GLU:HG2	2.00	0.42
1:C:255:TYR:O	1:C:259:THR:OG1	2.27	0.42
1:B:19:GLN:HA	1:B:53:VAL:O	2.19	0.42
1:A:179:ASN:O	1:A:180:TYR:C	2.63	0.42
1:B:242:HIS:CE1	2:B:301:36J:H17	2.54	0.42
1:C:27:VAL:HB	1:C:98:VAL:HG12	2.02	0.42
1:C:48:ALA:O	1:C:49:GLN:NE2	2.53	0.42
1:B:109:VAL:HG22	1:B:196:PRO:HG2	2.02	0.41
1:C:223:ASP:C	1:C:225:ILE:N	2.74	0.41
1:C:2:ARG:NH1	1:C:18:GLU:OE1	2.53	0.41
1:C:109:VAL:O	1:C:113:LEU:HB2	2.20	0.41
1:A:33:LEU:HG	2:A:300:36J:H9	2.01	0.41
1:A:221:PHE:O	1:A:222:PHE:C	2.62	0.41
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.86	0.41
1:A:37:GLN:HG2	1:A:172:VAL:CG2	2.51	0.41
1:C:38:MET:HE2	1:C:245:TYR:HE2	1.85	0.41
1:A:154:MET:HB3	1:A:165:TRP:CZ2	2.55	0.41
1:B:142:GLU:HG3	1:B:145:GLU:CD	2.45	0.41
1:B:202:ALA:O	1:B:206:LYS:HE2	2.21	0.41
1:B:242:HIS:CD2	2:B:301:36J:H5	2.56	0.41
1:C:252:PHE:CD1	1:C:252:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:O	1:C:225:ILE:N	2.54	0.40
1:B:34:GLY:O	1:B:57:ASP:HA	2.21	0.40
1:A:153:VAL:O	1:A:158:VAL:HG22	2.22	0.40
1:A:242:HIS:HB3	3:A:431:HOH:O	2.22	0.40
1:C:108:VAL:HA	1:C:111:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	244 (93%)	14 (5%)	4 (2%)	8	28
1	B	262/264 (99%)	246 (94%)	13 (5%)	3 (1%)	11	36
1	C	127/264 (48%)	103 (81%)	20 (16%)	4 (3%)	3	12
All	All	651/792 (82%)	593 (91%)	47 (7%)	11 (2%)	7	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
1	C	49	GLN
1	B	142	GLU
1	C	20	GLU
1	C	37	GLN
1	C	224	ASN
1	A	62	SER
1	A	161	GLY
1	B	161	GLY
1	A	187	TYR
1	B	187	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/220 (100%)	193 (88%)	27 (12%)	4	16
1	B	220/220 (100%)	194 (88%)	26 (12%)	5	17
1	C	126/220 (57%)	100 (79%)	26 (21%)	1	4
All	All	566/660 (86%)	487 (86%)	79 (14%)	3	12

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	41	SER
1	A	71	THR
1	A	82	SER
1	A	85	ILE
1	A	88	LEU
1	A	111	LEU
1	A	113	LEU
1	A	121	ASN
1	A	129	THR
1	A	131	LEU
1	A	135	LEU
1	A	136	SER
1	A	141	LEU
1	A	150	LEU
1	A	159	SER
1	A	163	GLU
1	A	182	VAL
1	A	190	THR
1	A	191	ILE
1	A	197	VAL
1	A	200	LEU
1	A	203	LEU
1	A	235	ILE
1	A	238	LEU
1	A	257	VAL

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Mol	Chain	Res	Type
1	A	262	LYS
1	B	22	THR
1	B	76	THR
1	B	84	VAL
1	B	85	ILE
1	B	88	LEU
1	B	99	TRP
1	B	109	VAL
1	B	113	LEU
1	B	121	ASN
1	B	131	LEU
1	B	136	SER
1	B	159	SER
1	B	163	GLU
1	B	172	VAL
1	B	176	LEU
1	B	189	ARG
1	B	190	THR
1	B	191	ILE
1	B	200	LEU
1	B	203	LEU
1	B	234	ASN
1	B	235	ILE
1	B	251	VAL
1	B	257	VAL
1	B	261	GLN
1	B	262	LYS
1	C	1	MET
1	C	2	ARG
1	C	25	ASP
1	C	31	ASP
1	C	37	GLN
1	C	38	MET
1	C	49	GLN
1	C	70	GLU
1	C	73	THR
1	C	82	SER
1	C	88	LEU
1	C	94	LYS
1	C	103	SER
1	C	111	LEU
1	C	113	LEU

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Mol	Chain	Res	Type
1	C	124	CYS
1	C	197	VAL
1	C	200	LEU
1	C	203	LEU
1	C	216	THR
1	C	223	ASP
1	C	225	ILE
1	C	227	THR
1	C	234	ASN
1	C	237	LEU
1	C	245	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	152	ASN
1	A	156	ASN
1	A	166	GLN
1	A	177	HIS
1	A	261	GLN
1	B	45	GLN
1	B	137	ASN
1	B	152	ASN
1	B	156	ASN
1	B	166	GLN
1	B	177	HIS
1	B	261	GLN
1	C	121	ASN
1	C	125	HIS
1	C	263	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	36J	B	301	-	24,24,24	1.48	4 (16%)	32,32,32	1.39	5 (15%)
2	36J	A	300	-	24,24,24	1.59	4 (16%)	32,32,32	1.25	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	36J	B	301	-	-	12/22/22/22	0/2/2/2
2	36J	A	300	-	-	9/22/22/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	36J	CAT-CAG	-4.54	1.39	1.47
2	A	300	36J	CAU-CAQ	-4.47	1.40	1.50
2	B	301	36J	CAT-CAG	-4.37	1.40	1.47
2	B	301	36J	CAU-CAQ	-3.98	1.41	1.50
2	B	301	36J	CAG-CAF	2.58	1.39	1.31
2	A	300	36J	CAG-CAF	2.54	1.39	1.31
2	A	300	36J	OAP-CAV	-2.04	1.43	1.47
2	B	301	36J	CAJ-CAF	-2.00	1.39	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	36J	CAV-OAP-CAQ	-3.07	111.94	117.67
2	B	301	36J	OAD-CAS-CAU	-2.89	115.79	121.14
2	A	300	36J	CAA-CAV-CAM	-2.74	106.81	113.90
2	B	301	36J	CAT-CAG-CAF	-2.63	120.00	125.55
2	A	300	36J	OAD-CAS-CAU	-2.60	116.34	121.14
2	A	300	36J	CAJ-CAF-CAG	-2.45	120.06	125.48
2	B	301	36J	CAN-CAK-CAJ	-2.44	109.18	114.47
2	A	300	36J	CAK-CAN-CAW	-2.41	108.04	114.68
2	B	301	36J	CAA-CAV-CAM	-2.27	108.02	113.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

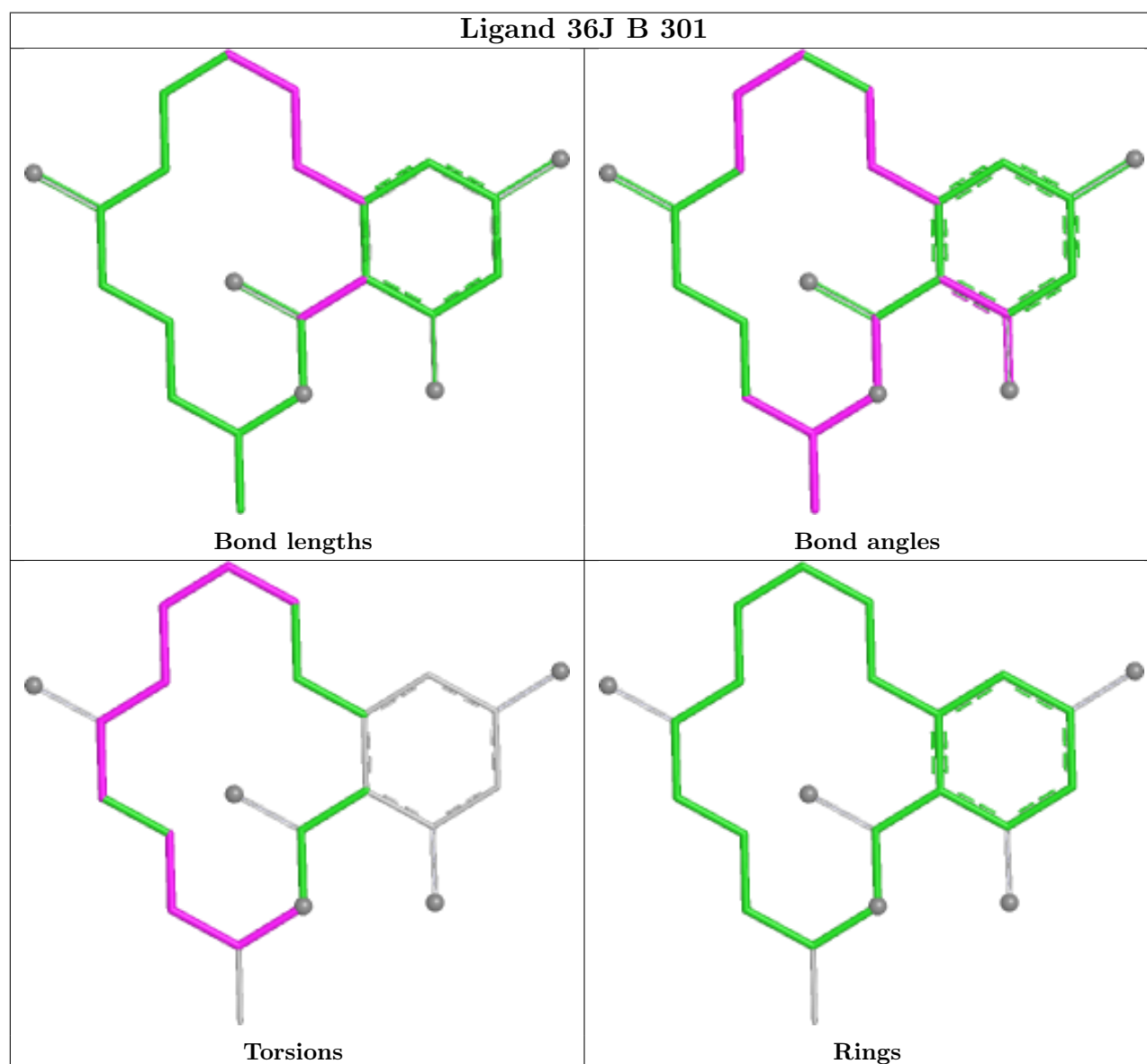
Mol	Chain	Res	Type	Atoms
2	A	300	36J	CAA-CAV-OAP-CAQ
2	A	300	36J	CAK-CAN-CAW-CAO
2	A	300	36J	CAK-CAN-CAW-OAE
2	B	301	36J	CAM-CAV-OAP-CAQ
2	B	301	36J	CAL-CAM-CAV-CAA
2	B	301	36J	CAL-CAM-CAV-OAP
2	A	300	36J	CAF-CAJ-CAK-CAN
2	B	301	36J	CAF-CAJ-CAK-CAN
2	B	301	36J	CAA-CAV-OAP-CAQ
2	B	301	36J	CAL-CAO-CAW-OAE
2	B	301	36J	CAK-CAN-CAW-CAO
2	A	300	36J	CAL-CAO-CAW-CAN
2	B	301	36J	CAO-CAL-CAM-CAV
2	B	301	36J	CAG-CAF-CAJ-CAK
2	B	301	36J	CAK-CAN-CAW-OAE
2	B	301	36J	CAL-CAO-CAW-CAN
2	A	300	36J	CAL-CAO-CAW-OAE
2	B	301	36J	CAJ-CAK-CAN-CAW
2	A	300	36J	CAM-CAV-OAP-CAQ
2	A	300	36J	OAP-CAQ-CAU-CAT
2	A	300	36J	OAP-CAQ-CAU-CAS

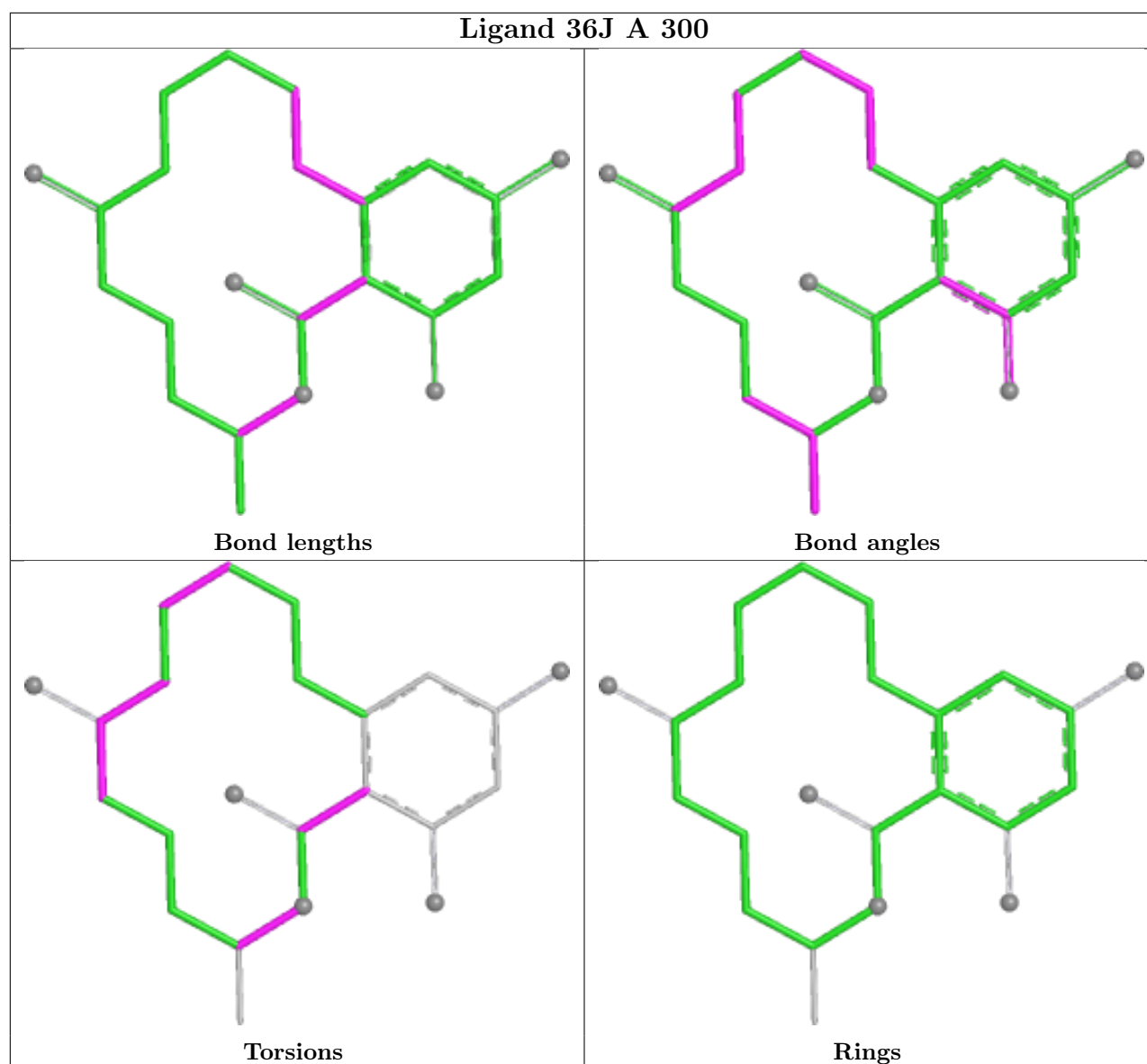
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	36J	7	0
2	A	300	36J	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/264 (100%)	-0.28	5 (1%) 66 57	12, 20, 44, 92	0
1	B	264/264 (100%)	-0.23	4 (1%) 72 63	14, 22, 50, 77	0
1	C	151/264 (57%)	1.63	48 (31%) 1 1	51, 74, 97, 131	0
All	All	679/792 (85%)	0.17	57 (8%) 17 12	12, 24, 84, 131	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	6.0
1	A	158	VAL	5.7
1	B	158	VAL	5.2
1	A	159	SER	4.5
1	C	203	LEU	4.3
1	C	237	LEU	3.8
1	C	109	VAL	3.7
1	C	242	HIS	3.5
1	C	251	VAL	3.5
1	C	192	PRO	3.5
1	B	157	ASP	3.4
1	C	69	PRO	3.4
1	C	247	SER	3.2
1	C	96	ALA	3.2
1	A	160	GLY	3.1
1	C	18	GLU	3.0
1	C	253	ALA	3.0
1	C	197	VAL	3.0
1	C	252	PHE	3.0
1	C	225	ILE	2.9
1	C	113	LEU	2.8
1	C	241	MET	2.7
1	C	216	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	88	LEU	2.7
1	C	98	VAL	2.7
1	C	72	TYR	2.7
1	C	231	ALA	2.6
1	C	99	TRP	2.6
1	C	209	ASP	2.6
1	C	104	GLY	2.5
1	B	159	SER	2.5
1	C	27	VAL	2.5
1	A	48	ALA	2.5
1	C	248	HIS	2.5
1	C	102	ALA	2.5
1	C	196	PRO	2.4
1	C	228	ALA	2.4
1	C	229	THR	2.4
1	C	256	VAL	2.3
1	C	246	VAL	2.3
1	C	257	VAL	2.3
1	C	217	PRO	2.3
1	A	157	ASP	2.3
1	C	245	TYR	2.2
1	C	32	GLY	2.2
1	C	215	ALA	2.2
1	C	238	LEU	2.2
1	C	1	MET	2.2
1	C	111	LEU	2.2
1	C	239	PRO	2.1
1	C	54	THR	2.1
1	C	15	TRP	2.1
1	C	30	PRO	2.1
1	C	112	LEU	2.1
1	C	100	GLY	2.0
1	B	139	ALA	2.0
1	C	38	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

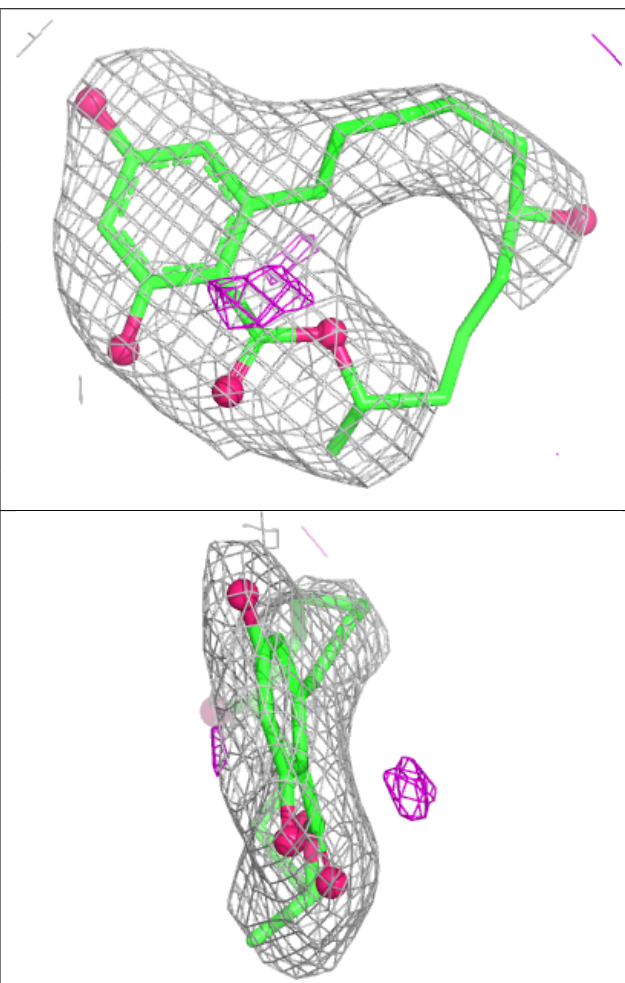
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	36J	B	301	23/23	0.92	0.15	44,54,80,85	0
2	36J	A	300	23/23	0.94	0.18	40,59,72,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

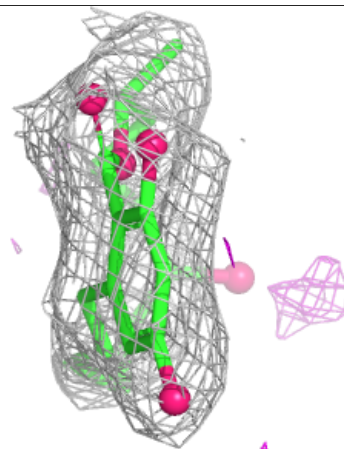
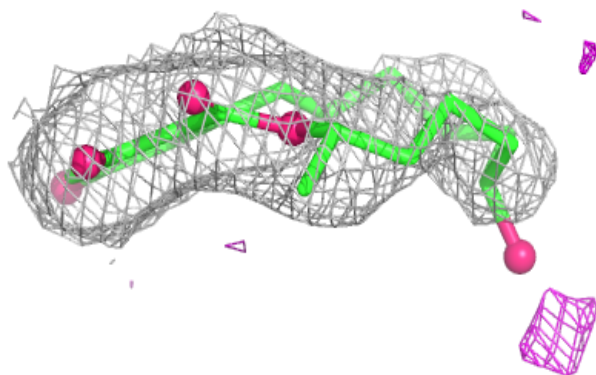
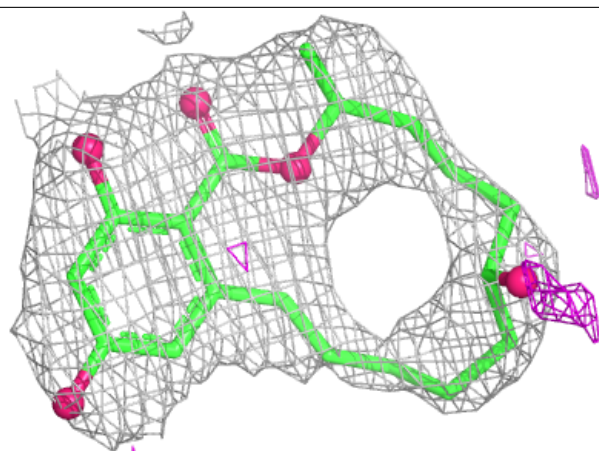
Electron density around 36J B 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 36J A 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.